SELF-CONSISTENT CALCULATIONS OF THE ISOTHERMAL ELASTIC CONSTANTS OF THE ANHARMONIC RARE-GAS CRYSTALS

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The reduced second-order self-consistent phonon approximation is applied to the calculations of the isothermal elastic constants of the anharmonic rare-gas crystals. As the models of nearest-neighbour central force interaction are used the Morse, Rydberg and Varshni self-consistent potentials. The temperature dependence of the isothermal elastic constants, bulk moduls and Grüneisen constants in the low and high temperature limits are given and compared with experimental data as well as with previous theoretical calculations.

Introduction

The principal theoretical results concerning the temperature dependence of the elastic constants $c_{\alpha\beta}$ of the ideal rare-gas crystals (RGC) in the quasi-harmonic (Q-H) approximation have been presented and discussed in [1, 2]. The results given in [2] for Ar, Kr and Xe in terms of the (12, 6) Lennard-Jones (L-J) potential showed that the Q-H approximation was unreliable for $T \gtrsim \frac{1}{3} T_m$ — the melting temperature.

Using the method of BARRON and KLEIN [3] and the pair potential function of BOBETIC—BARKER (B-B) [4] together with the AXILROD-TELLER triple-dipole interaction [5] BARKER and KLEIN calculated the harmonic and anharmonic elastic constants and phonon dispersion curves for Ar at low temperatures [4]. The phonon dispersion curves were in good agreement with experiment, but $c_{\alpha\beta}$ showed substantial differences from current experimental estimates.

An improved description of the elastic constant [7, 8], compared to the Q-H approximation, has been obtained in the lowest order self-consistent phonon theory (ISC) [9]. As the potential energy of the solid Ar the L-J potential was taken. However the ISC theory is known to be adequate up to about $\frac{3}{4}$ times of the melting temperature [10] so that up to this temperature the above calculations were performed.

Monte Carlo method with the B-B and L-J pair potentials was used to the calculations of the elastic constants of solid Ar, Kr and Xe in paper [11]. The results

for Ar (80 K) and Kr (85 and 115 K) have been obtained for the B-B pair potential. For Ar (80 K) and Xe (156 K) carried out the calculations for the L-J potential. The results obtained agreed well with the previous work of KLEIN and coworkers [8].

The self-consistent phonon theory based on the thermodynamic double-time Green's function method [12] was applied to the investigations of the isothermal elastic constants of the RGC in [13, 14]. The results reported there by graphs only were obtained for the Morse renormalized potential in the case of the displacement-displacement correlation function calculated at $T=0$.

Recently, the isothermal elastic constants of the RGC at $T=0$ K have been computed in terms of a new potential energy curve proposed by SINGH and NEB [15]. The agreement between experimental and theoretical results for $c_{\alpha\beta}$ was reasonably good. Singh's and Neb's paper does not contain investigation of the phonon properties from their new model of the potential energy curve.

In this paper, using the self-consistent phonon theory in the reduced second-order (RSC2) approximation [12,16], we show the anharmonic effects of phonons in the dynamic properties of the RGC. The calculations of the isothermal elastic constants, bulk modulus B and Grüneisen constants γ in terms of the Morse (M), Rydberg (R) and Varshni (V) self-consistent (*sc*) potentials are extended from low to high temperatures. For these potentials we can obtain explicit solutions of self-consistency equations for $c_{\alpha\beta}$ and for thermodynamical functions in analytical forms [17], which help to clarify some aspects of the theory of solid state. In order to assure the accuracy of the present calculations we used the parameters of the M, R and V potentials determined in higher approximation with respect to the number of shells n of nearest neighbours (N N) by the help of method described in [18]. Numerical values of these parameters for the RGC are listed in paper [19]. It should be noted, that M, R and V *sc* potentials used in recent our papers [19, 20] to the description of the thermodynamic properties of strongly anharmonic crystals gave reasonably good agreement with their measured as well as other theoretical data.

Isothermal Elastic Constants in the RSC2 Approximation

As was shown in [13] the isothermal elastic constants of the face-centred cubic crystals at temperature T and external pressure p are given by:

$$c_{\alpha\beta} = c^0_{\alpha\beta}\frac{r_e}{l}\alpha^2(T,p)[1-2\theta\beta(T,p)S_{k,j}], \tag{1}$$

where:

$c^0_{\alpha\beta}$ are the harmonic elastic constants,

r_e and l are the distance between neighbouring atoms in the harmonic and anharmonic approximations, respectively, $\alpha(T,p)$ and $\beta(T,p)$ are defined by the anharmonic strength constants $f(T,p)$ and $g(T,p)$.

$$\alpha^2(T,p) = \frac{f(T,p)}{f}, \tag{2}$$

$$\beta(T,p) = \frac{g^2(T,p)}{f^3(T,p)}. \tag{3}$$

$\theta = k_B T$, f is the harmonic force constants. The function $S_{\tilde{k},j}$ is defined by the appropriate choice of the type of the mode j and the direction $\tilde{k}$ of the wave vector yielding the corresponding elastic constants c_{11}, c_{44} and $c_{11}-c_{12}$ [13, 14]. ($S_{\tilde{k},j}$ evaluated in [14] are equal to: $S_{k_1 L}=1.73\times10^{-3}$, $S_{k_1 T}=1.36\times10^{-3}$ and $S_{k_2 T_2}=1.05\times10^{-2}$).

Analytical expressions for l, $\alpha(T,p)$ and $\beta(T,p)$ in terms of the Morse, Rydberg and Varshni *sc* potentials are given in paper [17]. We shall not collect here the analytical results of [17] but applying them to the lattices of Ne^{20}, Ar, Kr and Xe we will explore the temperature dependence of the isothermal elastic constants (Eq. (1)), bulk modulus [6]:

$$B = \frac{1}{3}(c_{11}+2c_{12}) \tag{4}$$

and Grüneisen constants [21]:

$$\gamma = \frac{\alpha_v V B}{C_v}, \tag{5}$$

where α_v, V and C_v are the coefficient of the volume thermal expansion, the volume of the crystal and the molar heat at constant volume, respectively. It should be noted that at $T=0\,\mathrm{K}$ γ has been calculated by the help of the expression given in paper [15].

The anisotropy A and parameter δ expressing the deviation from the Cauchy relation [6]:

$$A = 2c_{44}/(c_{11}-c_{12}), \tag{6}$$

$$\delta = (c_{44}-c_{12})/c_{11} \tag{7}$$

are computed too.

Numerical Results

The values of the isothermal elastic constants $c_{\alpha\beta}$ of the RGC calculated for the Morse, Rydberg and Varshni self-consistent potentials at $T=0\,\mathrm{K}$ are given in Table I. For comparison in this table are listed the experimental [22—24] and theoretical data obtained in terms of the LENNARD-JONES [2, 7, 26], BUCKINGHAM [26], BOBETIC-BARKER .4] and SINGH-NEB [15] potentials.

Numerical results for the bulk modulus B, anisotropy A and parameter δ obtained on the basis of the results of Table I are collected in Table II.

The temperature dependence of the isothermal elastic constants calculated in the RSC2 approximation are shown and compared with experimental [11, 22—24, 27—29] and other theoretical data [7, 11] in Table III and graphically in Figs 1—4.

Table IV shows the comparison of our results with the experimental [21, 33, 34] and theoretical data [10, 15, 32] for the Grüneisen constants γ as a function of temperature.

From Table I we can see that the agreement between experimental and our theoretical results for c_{11}, $c_{11}-c_{12}$ and c_{44} at $T=0\,\mathrm{K}$ is reasonably good. The harmonic elastic constants $c^0_{\alpha\beta}$ (appearing in Eq. (1)) have been calculated in terms of the M, R and V potentials on the basis of the Barron and Klein expressions [3]. The values of $c_{\alpha\beta}$ obtained in the RSC2 approximation are lower than those in the harmonic and Q-H approximations because the phonon frequency renormaliza-

Table I

Comparison on the values of the isothermal elastic constants calculated in terms of the Morse (M), *Rydberg* (R) *and Varshni* (V) *selfconsistent potentials with experimental* [22–25] *and theoretical data* [3, 6, 7, 15, 26] *obtained for the Lennard–Jones* (L–J), *Buckingham* (B), *Bobetic–Barker* (B–B) *and Singh–Neb* (S–N) *potentials at* $T=0$ K

Solids	Potential	Approximation	$c_{11}10^9$[Pa]	$(c_{11}-c_{12})10^9$[Pa]	$c_{44}10^9$[Pa]	Ref.
1	2	3	4	5	6	7
Ne	M	RSC2	1.136	0.547	0.692	
	R		1.303	0.617	0.805	
	V		1.323	0.648	0.793	
	L–J	Q–H	1.36	0.655	0.828	[3]
		ISC	1.597		0.825	[7]
	S–N	H*	1.334	0.350	0.498	[15]
	experim.	I N S**	1.611	0.756	0.972	[22]
Ar	M	RSC2	3.503	1.549	2.030	
	R		3.934	1.840	2.176	
	V		3.755	2.002	1.860	
	L–J	Q–H	3.71	1.64	2.15	[3]
		H	3.455	1.978	1.941	[26]
		ISC	3.978	2.012	2.600	[7]
	B–B	H	3.50	1.74	2.12	[6]
	B–B+ A–T***	H	3.79	1.73	2.12	
	B	H	4.069	2.413	2.366	[26]
	S–N	H	3.244	1.156	1.797	[15]
	experim.	I N S	4.24	1.85	2.250	[23]
Kr	M	RSC2	4.288	1.828	2.508	
	R		4.921	2.380	2.500	
	V		4.504	2.163	2.406	
	L–J	Q–H	4.52	1.97	2.60	[3]
		H	4.279	2.508	2.376	[26]
		ISC	4.876	2.451	3.220	[7]
	B	H	5.011	2.946	2.815	[26]
	S–N	H	4.236	1.547	2.500	[15]
	experim.	I N S	5.140	2.300	2.68	[24]
Xe	M	RSC2	5.012	2.177	2.874	
	R		5.234	2.321	2.853	
	V		5.150	2.425	2.575	
	L–J	Q–H	5.11	2.20	2.93	[3]
		H	4.715	2.78	2.592	[26]
		ISC	5.481	2.75	3.632	[7]
	B	H	5.505	3.261	3.067	[26]
	S–N	H	4.823	1.744	2.930	[15]
	experim.	I N S	5.270	2.45	2.950	[25]

* Harmonic approximation, ** inelastic neutron scattering method, *** Babetic–Baker potential together with the Axilrod–Teller triple-dipole interaction.

Table II

Bulk modulus B, anisotropy A and parameter δ of the RGC at T=0 K. The meaning of symbols is the same as in Table I

Solids	Potential	Approximation	$B\ 10^9$ [Pa]	A	δ
1	2	3	4	5	6
Ne	M	RSC2	0.771	2.55	0.175
	L-J	Q-H	0.923	2.528	0.174
		ISC			
	S-N	H	1.201	2.846	−0.521
	experiment		1.107	2.671	0.137
Ar	M	RSC2	2.470	2.621	0.039
	L-J	Q-H	2.617	2.620	0.038
		ISC	2.636	2.584	0.322
	B-B+A-T	H	2.636	2.450	0.029
	B	H	2.460	1.961	0.429
	S-N	H	2.473	3.109	−0.139
	experiment		3.020	2.432	− 0.054
Kr	M	RSC2	3.069	2.744	0.019
	L-J	Q-H	3.206	2.639	0.019
		ISC	3.242	2.627	0.328
	B	H	3.047	1.911	0.363
	S-N	H	3.205	3.232	−0.068
	experiment		3.607	2.330	−0.056
Xe	M	RSC2	3.561	2.640	0.019
	L-J	Q-H	3.643	2.663	0.020
		ISC	3.647	2.641	0.328
	B	H	2.862	1.865	0.363
	S-N	H	3.660	3.360	−0.068
	experiment		3.636	2.407	−0.056

tion factor $\alpha<1$ and $l>r_e$ even at $T=0$ K. In addition, at sufficiently high temperature the differences between numerical values of our results for $c_{\alpha\beta}$ and those in the ISC theory are due to the negative contributions from the second order terms in the self-energy operator $(-\beta(T,p)$ in Eq. (1)). It is worthwhile to underline that the contributions from the odd-derivative terms in the *sc* potential which describe the damping of phonons lead to a decrease of the numerical values of some thermodynamical functions [17] and instability temperature [20] of the crystals also.

The Grüneisen constants calculated from our self-consistent potentials are essentially temperature independent. This conclusion is in agreement with experimental data for Kr and Xe in high temperature limit. Approximately this conclusion concerns the values of γ computed by KLEIN and co-workers [10]. Let us remind here that γ obtained in paper [10] for Ar in the case of the Bobetic–Barker and Barker–Fisher–Watts potentials at $T=20-60$ K are in the range of 2.9—3.0 and of 2.8—2.9, respectively.

Table III

Comparison of the experimental and theoretical data for the isothermal elastic constants as a function of temperature. The meaning of symbols is the same as in Table I

Solids	Potential	T [K]	c_{11} 10^9 [Pa]	c_{12} 10^9 [Pa]	c_{44} 10^9 [Pa]	Ref.
1	2	4	4	5	6	7
Ne	M	5	1.113	0.577	0.678	
		24	0.946	0.490	0.542	
	R	5	1.283	0.675	0.792	
		24	1.091	0.573	0.633	
	V	5	1.296	0.661	0.777	
		24	1.102	0.562	0.621	
	L–J	7	1.588		0.821	[7*]
	(ISC)	23.5	1.112		0.597	
	experiment	5	1.661 ± 0.017	0.855 ± 0.021	0.952 ± 0.05	[22]
Ar	M	10	3.433	1.915	1.986	
		80	2.059	1.149	1.192	
	R	10	3.855	2.052	2.121	
		80	2.313	1.231	1.272	
	V	10	3.679	1.718	1.822	
		80	2.207	1.031	1.093	
	L–J	10	3.958		2.003	[7*]
	(ISC)	83	2.147		1.148	
	L–J (Monte C.)	80*	1.917	0.92	2.20	[11]
	B–B (Monte C.)	80*	1.91	1.03	1.18	[11]
		10	4.25 ± 0.05	2.40 ± 0.05	2.24 ± 0.01	[23]
	experiment	80	2.14	0.83	0.89	[11]
		82	2.48 ± 0.06	1.53 ± 0.05	1.24 ± 0.04	[23]
Kr	M	10	4.159	2.386	2.432	
		115	2.495	1.432	1.459	
	R	10	4.773	2.464	2.425	
		115	2.864	1.478	1.455	
	V	10	4.368	2.271	2.333	
		115	2.621	1.362	1.400	
	L–J	10	4.84		2.434	[7*]
	(ISC)	115	2.50		1.331	
	B–B (Monte C.)	85*	2.88	1.57	1.72	[11]
		115*	2.05	1.16	1.27	
	experiment	10	5.21 ± 0.05	2.92 ± 0.06	2.68 ± 0.03	[24]
		85*	3.24	1.1	1.63	[11]
		114	2.89 ± 0.04	1.85 ± 0.04	1.44 ± 0.01	[27]
		114	2.99	1.07	1.19	[28]
		115*	2.38		1.19	[11]
Xe	M	10	4.841	2.749	2.787	
		110	2.917	1.650	1.672	
		156	2.041	1.154	1.171	
	R	10	5.076	2.825	2.767	
		110	3.046	1.695	1.660	
		156	2.132	1.186	1.162	
	V	10	4.995	2.643	2.497	
		110	2.997	1.585	1.438	

Table III

(Continued)

1	2	3	4	5	6	7
		156	2.098	1.110	1.049	
	L–J	160	2.806		1.49	[7*]
	(ISC)					
	(Monte C.)	156*	2.14	1.18	1.48	[11]
Xe	experim.	10	5.27±0.09	2.82±0.08	2.95±0.04	[29]
		110	4.14±0.06	2.40±0.06	2.11±0.04	
		159.6	2.83±0.05	1.73±0.05	1.50±0.02	
		156*	2.30	1.22	1.48	[11]
		156	2.12	1.04	1.48	[30]

The values of $c_{\alpha\beta}$ obtained on the basis of the relation [31]: $c_{\alpha\beta}-c^S_{\alpha\beta}=B-B^S$, where $c^S_{\alpha\beta}$ and B^S are the adiabatic elastic constants and adiabatic bulk modulus, respectively. $\alpha=1$, $\beta=1.2$.

Table IV

Temperature dependence of the experimental and theoretical values of the Grüneisen constants γ

Solids	T [K]	Experiment	M	R	V	S-N [15]	B-B [10]	L-J [32]
	0	3.1 [21]	3.031	3.029	3.017	2.10		3.22
	8		3.031	3.029	3.017			
Ne	16		3.031	3.030	3.018			
	24	3.5	3.094	3.052	3.033			
	0	2.8 [21]	2.880	2.501	2.416	2.063		3.10
	20	3.10 [33]	2.897	2.851	2.512		2.9	
Ar	40	2.81	2.941	2.947	2.626			
	50	3.1 [21]	2.966	2.974	2.837			
	70		3.044	2.967	2.967		3.0	
	0	2.75 [21]	2.612	2.611	2.614	2.532		2.80
	20	2.77 [34]	2.619	2.623	2.629			
Kr	60	2.84	2.655	2.662	2.683			
	100	2.81	2.719	2.709	2.738			
	115	2.81	2.743	2.747	2.747			
	0	2.75 [21]	2.808	2.812	2.810	1.948		2.87
	20		2.804	2.813	2.815			
Xe	60	2.72 [33]	2.843	2.847	2.852			
	100	2.9	2.896	2.886	2.892			
	120	3.0	2.897	2.902	2.908			
	140	3.1	2.919	2.925	2.932			

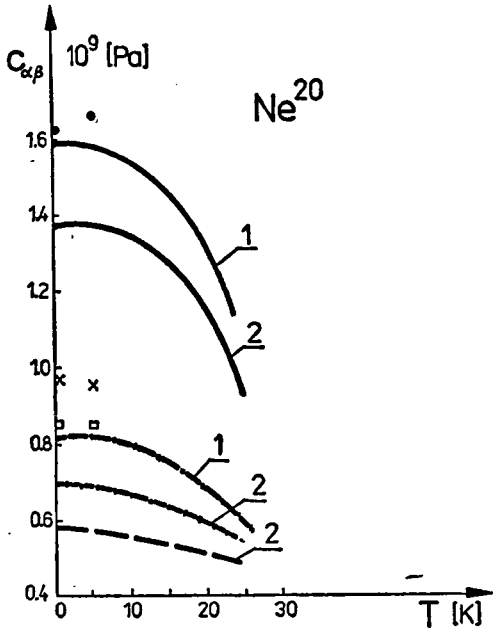

Fig. 1. Temperature dependence of the isothermal elastic constants of Ne^{20} for the Morse self-consistent potential in the RSC2 approximation (curves 2) and for the (12,6) Lennard-Jones potential energy function in the ISC theory [7*] (curves 1).
c_{11}(————); c_{12}(— —);
c_{44}(—·—·—·—).
The experimental data [22] are shown by:
c_{11}— ● ●; c_{12}— □ □;
c_{44}— × ×, respectively

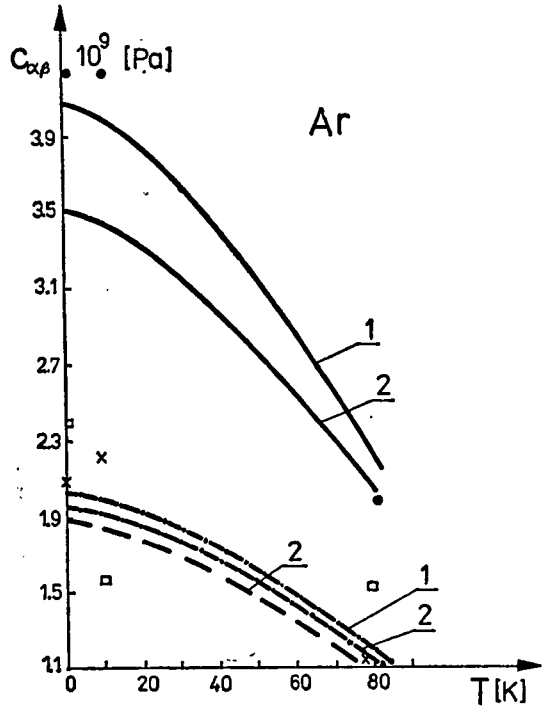

Fig. 2. Temperature dependence of the isothermal elastic constants for Ar. The meaning of curves is the same as in Fig. 1. The experimental data are from measurements of [11, 23]

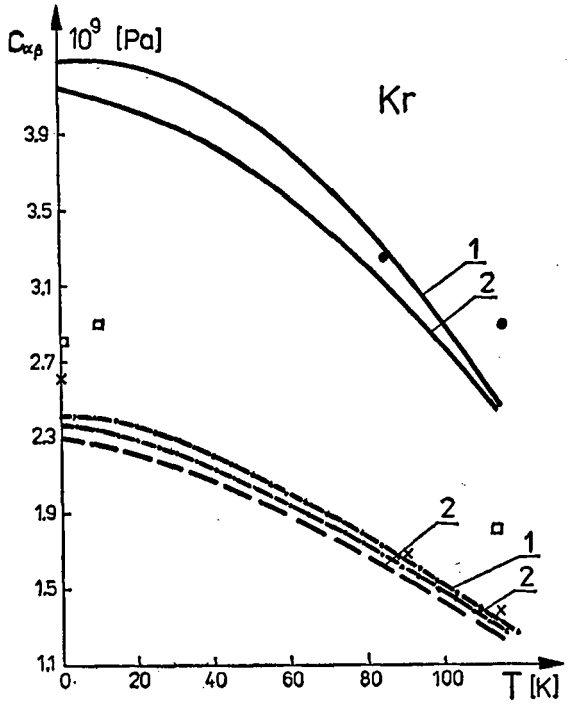

Fig. 3. Temperature dependence of the isothermal elastic constants for Kr. The meaning of curves is the same as in Fig. 1. The experimental data are from measurements of [11, 24, 28, 30]

Conclusions

In conclusion we would like to mention that, considering the large number of properties [12—14, 16—20] investigated on the basis of the self-consistent phonon theory (SCPT) of anharmonic crystals developed by PLAKIDA and SIKLÓS [12, 16], the overall agreement with the experimental values may be said to be quite satisfactory. This paper presents a continuation of our investigation on the properties of cubic crystals in the SCPT. The calculations are performed in the reduced second-order SCPT using the Morse, Rydberg and Varshni renormalized potentials as models of nearest-neighbour central force interaction. The numerical results obtained for the isothermal elastic constants $c_{\alpha\beta}$, bulk modulus B and Grüneisen constants γ of the ideal rare-gas crystals (RGC) are compared with available experimental data as well as with principial theoretical results (Tables I, III and IV). From this comparative presentation the values of $c_{\alpha\beta}$ follows that our results are generally smaller than those obtained by the help of previous approximation. It is due to the contributions to $c_{\alpha\beta}$ from the add-derivative terms in the *sc* potential which describe

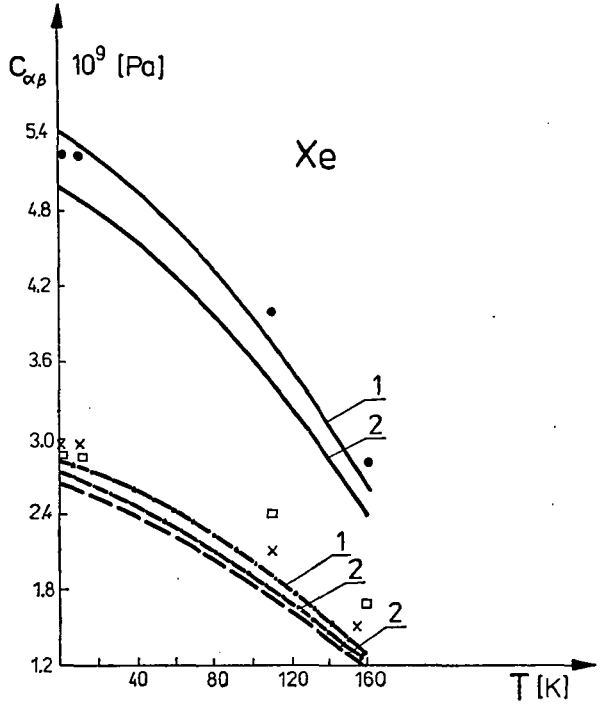

Fig. 4. Temperature dependence of the isothermal elastic constants for Xe. The meaning of curves is the same as in Fig. 1. The experimental data are from measurements of [29]

the damping of phonons. According to Eq. (1) these contributions come from two sources: i) the crystal expands as the temperature increases so that $r_e/l<1$, ii) our elastic constants include the negative contribution $(-\beta(T,p))$ from the second order term in the self-consistent theory which is neglected in the ISC approximation. Let us remind here that in the Q-H approximation the anharmonic effect in the elastic constants was represented by using the vibrational elongation that is defined by the average increase of the effective interatomic distances only [1].

It should be noted that the self-consistent potentials sufficiently differ from the interaction potentials in their harmonic approximations [20 b] so that l differs sufficiently from r_e and $c_{\alpha\beta}<c^0_{\alpha\beta}$ even at $T=0$ K.

The notable differences between experimental and our results for $c_{\alpha\beta}$ are attributable to the use of a simple models of renormalized potentials. Nevertheless, we hope that the present study shows that the second-order self-consistent phonon approximation gives a reasonably satisfactory description of the isothermal elastic constant of RGC.

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МОДУЛИ УПРУГОСТИ АНГАРМОНИЧЕСКИХ КРИСТАЛЛОВ ИНЕРТНЫХ ГАЗОВ В ТЕОРИИ САМОСОГЛАСОВАННОГО ПОЛЯ

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С учётом членов второго порядка самосогласованной теории вычислены модули упругости $c_{\alpha\beta}$, модули всестороннего сжатия B и параметры Грюнайзена γ ангармонических кристаллов инертных газов. Система самосогласованных уравнений, определяющих динамические величины кристаллов Ne, Ar, Kr и Xe в пределе низких и высоких температур, решена для парного центрального взаимодействия ближайших соседей апроксимированного кривыми Морзе, Ридберга и Варшни. Результаты вычислений $c_{\alpha\beta}$, B и γ хорошо совпадают с экспериментальными и другими теоретическими данными для аргона, криптона и ксенона.